# 2-Methylphenanthrene

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2531-84-2	DTXSID1	025649

## **Model Performance**

Marada I	D. L.
Model	Data
110001	Bata

# Weighted KNN model

5-fold CV (75%)		Training (	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

#### Model Results

Predicted value: 76.2 °C

Global applicability domain: Inside

Local applicability domain index: 1.00

Confidence level: 6.64e-01

## Nearest Neighbors from the Training Set

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9-Methylanthracene Measured: 81.5 Predicted: 80.3

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4-Methylphenanthrene Measured: 53.5 Predicted: 76.2

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1-Methyl phenanthrene Measured: 123 Predicted: 76.2

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3-Methylphenanthrene Measured: 65.0 Predicted: 76.2

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2-Methylphenanthrene Measured: 58.0 Predicted: 76.2